

Half-metallic ferrimagnetism in the $[Sc_{1-x}V_x]C$ and $[Sc_{1-x}V_x]Si$ alloys adopting the zinc-blende and wurtzite structures from first-principles

K. Özdoğan^aE. Şaşioğlu^{b,c}I. Galanakis^{d,*}

^a*Department of Physics, Gebze Institute of Technology, Gebze, 41400, Kocaeli, Turkey*

^b*Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany*

^c*Fatih University, Physics Department, 34500, Büyükçekmece, İstanbul, Turkey*

^d*Department of Materials Science, School of Natural Sciences, University of Patras, GR-26504 Patra, Greece*

Abstract

Employing first-principles calculations we study the structural, electronic and magnetic properties of the $[Sc_{1-x}V_x]C$ and $[Sc_{1-x}V_x]Si$ alloys. In their equilibrium rocksalt structure all alloys are non-magnetic. The zincblende and wurtzite structures are degenerated with respect to the total energy. For all concentrations the alloys in these lattice structures are half-metallic with the gap located in the spin-down band. The total spin moment follows the Slater-Pauling behavior varying linearly between the $-1 \mu_B$ of the perfect ScC and ScSi alloys and the $+1 \mu_B$ of the perfect VC and VSi alloys. For the intermediate concentrations V and Sc atoms have antiparallel spin magnetic moments and the compounds are half-metallic ferrimagnets. At the critical concentration, both $[Sc_{0.5}V_{0.5}]C$ and $[Sc_{0.5}V_{0.5}]Si$ alloys present zero total spin-magnetic moment but the C-based alloy shows a semiconducting behavior contrary to the Si-based alloys which is a half-metallic antiferromagnet.

Key words: Electronic structure, Half-metals, Ferrimagnets

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1. Introduction

Half-metallic ferromagnets have attracted considerable attention during the last decade due to their potential applications in magnetoelectronic devices [1]. The term “half-metal” was initially introduced by de Groot and collaborators in 1983 to denote the peculiar behavior exhibited by a Heusler compounds: NiMnSb [2]. They have found using first-principles calculations that the majority-spin band was metallic while the minority-spin band was semi-

conducting leading to 100% spin-polarization of the electrons at the Fermi level. This behavior was later confirmed both by infrared absorption [3] and by spin-polarized positron annihilation [4] experiments.

Although Heusler alloys have attracted a lot of interest as potential half-metallic systems, the discovery of Akinaga and his collaborators in 2000 has shown the possibility to grow new half-metallic systems in metastable structures usually adopted by thin films [5]. They have shown that the CrAs/GaAs multilayers are ferromagnets and surprisingly the X-ray diffraction measurements suggest that CrAs adopts the lattice structure of GaAs and grows in the metastable zincblende structure. Moreover SQUID measurements have shown that CrAs exhibits an integer total spin magnetic moment of $3 \mu_B$ per unit

* Corresponding author. Phone +30-2610-969925, Fax +30-2610-969368

Email addresses: kozdogan@gyte.edu.tr (K. Özdoğan), e.sasioglu@fz-juelich.de (E. Şaşioğlu), galanakis@upatras.gr (I. Galanakis).

cell [5]. These findings have intensified the interest on transition-metal pnictides and chalcogenides like CrAs and CrSe which crystallize either in the zinc-blende or wurtzite structures of binary semiconductors and an extended review can be found in reference [6]. Galanakis and Mavropoulos have studied using first-principles calculations several such compounds and have determined the lattice constants for which half-metallicity is present [7]. Moreover they have explained the gap in terms of the $p-d$ repulsion; the p orbitals of the sp atom hybridize with the t_{2g} orbitals of the transition metal atoms creating three bonding and three antibonding states. The gap is created between these states. The e_g orbitals of the transition metal atom are very localized in energy since they do not hybridize with other orbitals and they are placed above the Fermi level in the spin-down band. Their relative position with respect to the antibonding $p-t_{2g}$ orbitals depends on each system. It has been also shown in the same reference that except the three bonding $p-t_{2g}$ bands below the Fermi level exists also a deep s band. Thus, since there are exactly four spin-down occupied bands, the total spin moment, M_t , follows a Slater-Pauling behavior and it equals in μ_B units: $M_t = Z_t - 8$ where Z_t the total number of valence electrons in the unit cell.

As we mentioned above most of the studies concern cases where the sp atom belongs to the Vth (pnictides) or the VIth (chalcogenides) column of the periodical table. The case where the sp atom comes from the IVth column of the periodical table has attracted much less attention in literature and to the best of our knowledge only the cases of MnC [8,9,10], MnSn [9] and MnSi [11,12,13] in the zincblende lattice have been studied. In this manuscript we study using the full-potential nonorthogonal local-orbital minimum-basis band structure scheme (FPLO) [14] within the local density approximation (LDA) [15] the case of $[Sc_{1-x}V_x]C$ and $[Sc_{1-x}V_x]Si$ alloys for x taking the values 0, 0.1, 0.2, ..., 0.9, 1. The disorder is simulated using the coherent potential approximation [16]. ScC and ScSi compounds have 7 electrons per unit cell and, if they are half metals, they should show a total spin moment of $-1 \mu_B$. On the other hand VC and VSi have 9 electrons and, if they are half-metals, should exhibit a total spin moment of $+1 \mu_B$. Thus within these families of alloys we can study the transition at the $x = 0.5$ concentration where the total spin moment changes sign. In section 2 we study the perfect compounds to determine

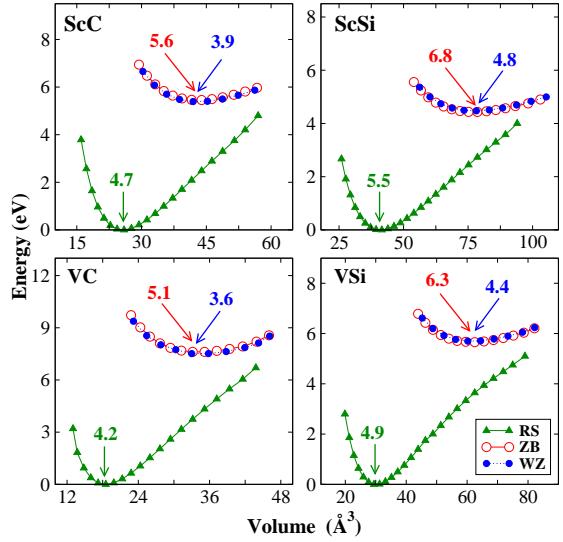


Fig. 1. (Color online) Calculated total energy as a function of the volume of the unit cell for ScC, ScSi, VC and VSi in the rocksalt (RS), zincblende (ZB) and wurtzite (WZ) structures. The zero of the total energy is defined as the energy of the global equilibrium volume and with arrows we represent the corresponding equilibrium lattice constant; for the WZ structure which is not cubic we give the in-plane lattice parameter a and the c/a ratio is for all calculations the ideal $(\frac{8}{3})^{\frac{1}{2}}$ for which the nearest environment in the WZ structure is the same with its cubic ZB analogue. In the RS and ZB there is one transition-metal atom and one sp atom per unit cell. In the WZ structure there are two atoms of each chemical kind but we have divided the energy by two to compare it directly to the other two cases.

the equilibrium lattice constants and we show that all four ScC, ScSi, VC and VSi crystallize in the non-magnetic rocksalt structure. In section 3 we continue our study with the case of the magnetic zincblende and wurtzite structures which are degenerated with respect to their total energy and we study both the electronic and magnetic properties. We show that for the intermediate concentrations the total spin moment scales linearly with the concentration and the Sc and V atoms have antiparallel spin magnetic moments. We also try to explain why for $x = 0.5$ the C-based alloy is a semiconductor while the Si-based alloys is a half-metallic antiferromagnet [17]. The latter property is highly desirable for applications since such materials create vanishing stray fields and thus minimize energy losses in devices. Finally in section 4 we summarize and present our conclusions.

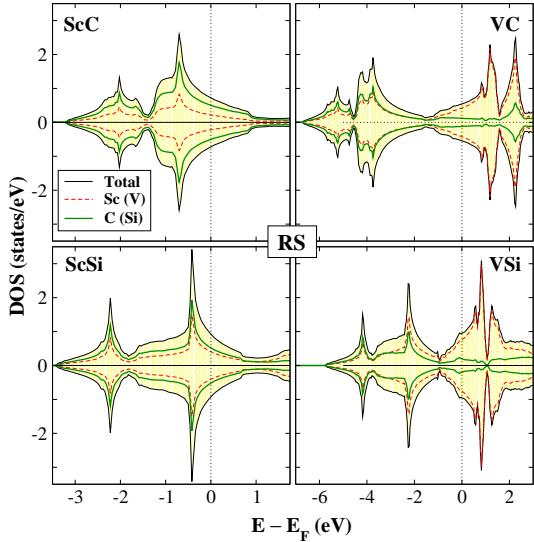


Fig. 2. (Color online) Total and atom-resolved density of states (DOS) for all four perfect compounds in the rock-salt structure at their equilibrium lattice constants. We present upwards the DOS for the spin-up states and downwards for the spin-down. In this structure we have converged to a non-magnetic state for all four alloys. The Fermi level has been chosen as the zero of the energy axis.

2. Total energy calculations

We will start the presentation of our results discussing the equilibrium lattices and lattice constants. We have taken into account three different lattices: (i) the rocksalt (RS), (ii) the zincblende, and (iii) the wurtzite (WZ) structures, and we present in figure 1 the calculated total energy as a function of the volume of the unit cell. Before proceeding with the discussion and presentation of our results we should focus on the characteristics of the three structures under study. We have chosen the RS structure since it is adopted by the majority of the binary compounds between transition-metal and *sp* atoms when the stoichiometry is 1:1. The lattice is actually a fcc with two atoms as basis set, one atom at $(0\ 0\ 0)$ and the second atom at $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$ in Wyckoff coordinates. Thus the RS is a close packed structure. Contrary to RS both ZB and WZ structures are open structures. In the ZB structure the lattice is again a fcc with four sites as basis set along the diagonal, but now two out of the four sites are empty. The WZ is the hexagonal analogue of the ZB structure. In our WZ calculations we have varied only the in-plane lattice parameter a and we have considered that the c/a ratio is for all calculations the ideal $(\frac{8}{3})^{\frac{1}{2}}$ for which the nearest

environment in the WZ structure is the same with its cubic ZB analogue. Finally we should mention that in the RS and ZB there is one transition-metal atom and one *sp* atom per unit cell while in the WZ structure there are two atoms of each chemical kind. We have divided in the WZ case by two all the properties, which are calculated per unit cell (total density of states, total spin magnetic moment and total energy), in order to compare them directly to the other two cases.

For all four perfect compounds presented in figure 1 the RS structure is the equilibrium lattice and the energy difference between the equilibrium RS lattice constant and the ZB-WZ equilibrium lattice constants is between 4 and 8 eV which are very large energy differences. Thus in the form of single crystals all ScC, ScSi, VC and VSi prefer to crystallize in the RS lattice. As expected the equilibrium volume is much smaller in the RS case compared to the other two since in the former one no voids exist. Surprisingly our results suggest that the ZB and WZ structure are degenerated in all cases and thus, when grown as thin films on top of semiconductors, the unit cell can easily deform itself. In the same figure we have also denoted the equilibrium lattice constants for all three structures (for the WZ one we give the in-plane lattice parameter). We remark that the trends depend on the chemical elements. When we substitute Si for C, the equilibrium lattice parameters increases. C and Si have both four valence electrons but C has six electrons in total (the atomic configuration is $1s^2\ 2s^2\ 2p^2$) while Si has 14 electrons (the atomic configuration is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$) and thus occupies more space. Sc and V belong in the same series in the periodic table. Sc has three valence electrons (the valence electrons in the atomic configuration are the $4s^2$ and $3d^1$) and V has two more *d* electrons and thus in total five valence electrons. Although V has more valence electrons than Sc, it is well known that for the early transition metal atoms as the valence increases the lattice parameter decreases [18] and this is also the cases here. VC and VSi correspond to smaller equilibrium lattice parameters than ScC and ScSi, respectively.

Finally we should discuss the electronic properties in the case of the RS structure before proceeding in the next section with the ZB and WZ structures. In the RS lattice all four perfect compounds are non-magnetic as can be seen from the density of states (DOS) presented in figure 2. In the case of the ScC and ScSi alloys the Fermi level crosses the valence band, which is created by the bonding states due to

the hybridization between the Sc d - and the C(Si) p -orbitals, and the atom-resolved DOS has a similar shape for both the Sc and C(Si) atoms. When we substitute V for Sc we populate also partially the conduction band created by the antibonding $p - d$ states. As can be seen in the figure, the conduction band has its main weight mainly at the vanadium atom since the latter one offers a lot of empty d -states with respect to the empty p states of the sp atoms. Finally we should note that for all four alloys there is one s band lying very deep in energy and which is separated by more than 3 eV from the bottom of the valence band and thus we do not present it in figure 2.

3. Ferrimagnetism in the zincblende and wurtzite structures

As we showed in the previous section all compounds under study are non-magnetic in the equilibrium RS lattice and thus are not useful for spintronic applications. Contrary to the RS case, we found all four ScC, ScSi, VC and VSi to be magnetic in both the ZB and WZ structures. Although these structures are not stable ones, it is possible to occur when these alloys are grown as thin films or multilayers on top of binary semiconductors adopting the same lattice structure. This is possible with the new up-to-date experimental techniques like Molecular Beam Epitaxy or Pulsed Layer Deposition and in fact the former method was employed to grow the CrAs films with the ZB structure on top of the GaAs semiconductor in reference [5].

We will start our discussion from the properties of the perfect compounds and in table 1 we have gathered the atom-resolved and total spin magnetic moments and in figure 3 we present the associated DOS. All presented calculations have been performed at the equilibrium lattice constants presented in figure 1. Our first remark concerns the difference between the ZB and WZ structures. As we can see in table 1, the spin magnetic moments only scarcely vary between the two lattice structures and the same occurs also for the total and atom-resolved DOS presented in figure 3 (note that we have divided the total spin moment and DOS in the WZ structure by two to make it comparable to the ZB case). Thus we will concentrate our discussion to the ZB case and refer to the WZ structure only if the difference with respect to the ZB lattice is significant. ScC has in total 7 valence electrons per unit cell and thus in

Table 1

Total and atom-resolved spin magnetic moments in μ_B for all compounds under study at the equilibrium lattice constants for the zincblende (ZB) and wurtzite (WZ) structures. For the intermediate concentrations we have considered that the lattice constant scales linearly with the concentration. We have scaled the atom-resolved spin moments to one atom. The total spin moment is the sum $(1 - x) * m^{Sc} + x * m^V + m^{C(Si)} + m^{int}$, where m^{int} refers to the interstitial region (empty sites). We do not present m^{int} separately since it is negligible with respect to the atomic spin moments. In the ZB there is one transition-metal atom and one sp atom per unit cell, while in the WZ structure there are two equivalent atoms of each chemical kind and thus we present half the total spin moment in the unit cell to compare it directly to the ZB case.

		[Sc _{1-x} V _x]C							
		zincblende				wurtzite			
x		m^{Sc}	m^V	m^C	m^{Total}	m^{Sc}	m^V	m^C	m^{Total}
0	-0.179	-	-0.821	-1.000		-0.186	-	-0.814	-1.000
0.1	-0.177	0.994	-0.740	-0.799		-0.201	1.122	-0.731	-0.800
0.2	-0.170	0.783	-0.620	-0.599		-0.202	0.968	-0.632	-0.600
0.3	-0.144	0.533	-0.458	-0.399		-0.183	0.764	-0.501	-0.400
0.4	~0	~0	~0	~0		-0.126	0.466	0.310	-0.200
0.5	~0	~0	~0	0		~0	~0	~0	0
0.6	-0.064	0.646	-0.162	0.200		-0.090	0.755	-0.217	0.200
0.7	-0.086	0.899	-0.204	0.400		-0.108	0.986	-0.258	0.400
0.8	-0.098	1.047	-0.218	0.600		-0.117	1.122	-0.274	0.600
0.9	-0.107	1.144	-0.219	0.800		-0.122	1.215	-0.282	0.800
1	-	1.192	-0.192	1.000		-	1.194	-0.194	1.000

		[Sc _{1-x} V _x]Si							
		zincblende				wurtzite			
x		m^{Sc}	m^V	m^{Si}	m^{Total}	m^{Sc}	m^V	m^{Si}	m^{Total}
0	-0.349	-	-0.651	-1.000		-0.367	-	-0.633	-1.000
0.1	-0.383	2.030	-0.658	-0.799		-0.403	1.868	-0.624	-0.800
0.2	-0.423	1.914	-0.644	-0.599		-0.436	1.778	-0.607	-0.599
0.3	-0.451	1.764	-0.613	-0.399		-0.457	1.656	-0.577	-0.399
0.4	-0.448	1.558	-0.554	-0.199		-0.456	1.504	-0.527	-0.199
0.5	-0.405	1.325	-0.460	-0.001		-0.429	1.352	-0.461	0.001
0.6	-0.413	1.324	-0.429	0.200		-0.417	1.308	-0.418	0.200
0.7	-0.426	1.333	-0.405	0.400		-0.414	1.302	-0.387	0.400
0.8	-0.439	1.337	-0.381	0.600		-0.413	1.305	-0.361	0.600
0.9	-0.451	1.335	-0.356	0.800		-0.414	1.310	-0.338	0.800
1	-	1.330	-0.330	1.000		-	1.288	-0.288	1.000

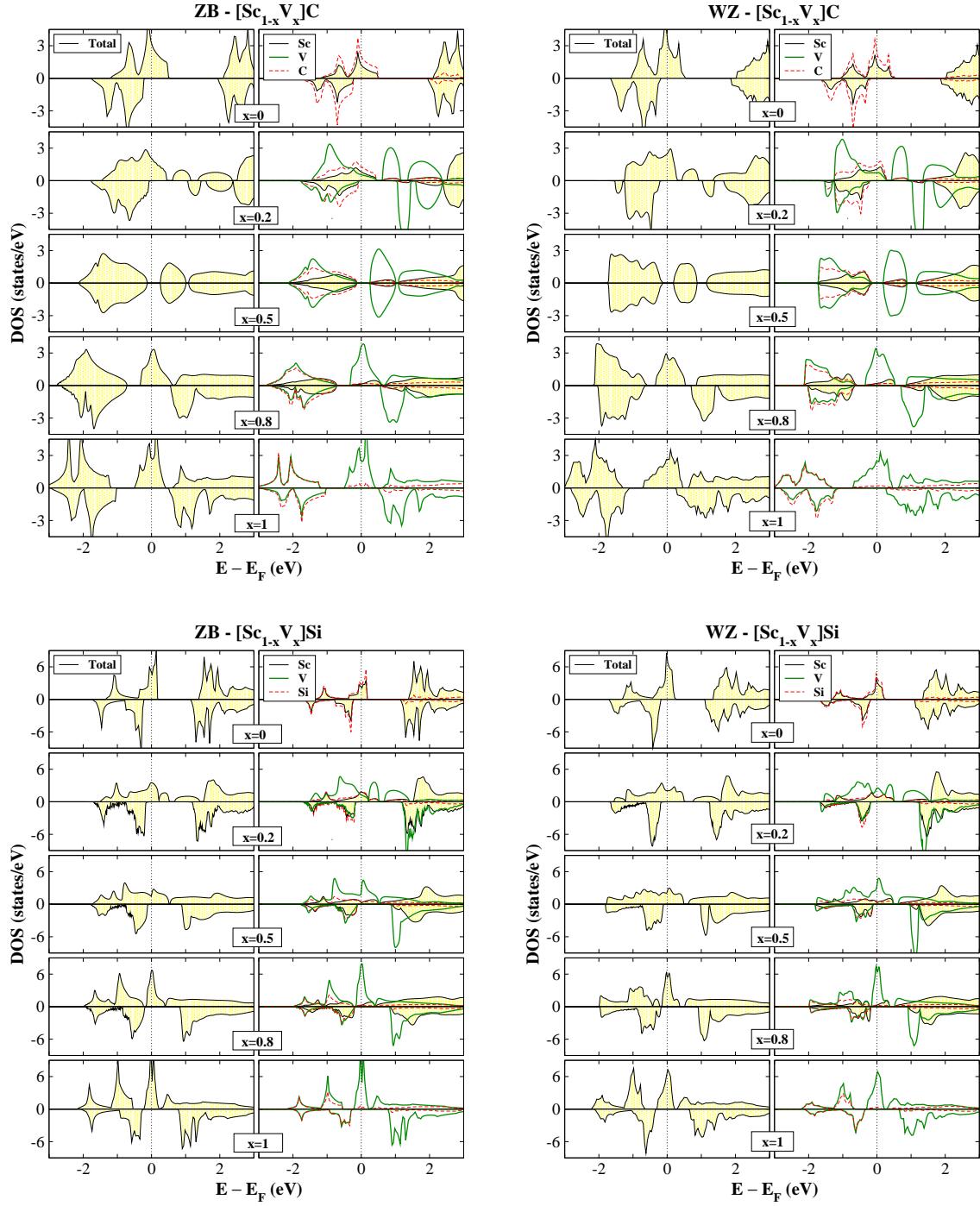


Fig. 3. (Color online) Total and atom-resolved DOS for $[Sc_{1-x}V_x]C$ (upper panel) and $[Sc_{1-x}V_x]Si$ (lower panel) in both zincblende (left) and wurtzite (right) lattice structures for several values of the concentration x . The lattice parameter has been assumed to vary linearly between the equilibrium lattice constants of the $ScC(ScSi)$ and $VC(VSi)$ alloys. We have scaled the atom-resolved DOS to one atom. In the case of the wurtzite structure the unit cell contains double the atoms of the zincblende unit-cell and thus we have scaled the total DOS in the wurtzite structure by 0.5 to make them comparable. In all cases the deep lying s states are not shown.

order to be half-metal it should exhibit a spin magnetic moment of $-1 \mu_B$ according to the $M_t = Z_t - 8$ Slater-Pauling rule. This is actually the case since, as can be seen in table 1, Sc carries a spin moment of around $-0.18 \mu_B$ and C atoms carry a spin moment of around $-0.82 \mu_B$. Although it seems strange that the spin moment is mainly concentrated to the sp atoms, this phenomenon can be easily understood if we look at the DOS in figure 3. In the spin-down band all four states are occupied. These states, as we have already discussed in section 1 and as it is shown in reference [7], consist of a deep lying s -state and three bonding states due to the hybridization between the p electrons of the C and the t_{2g} d -electrons of the Sc atom. These bonding states are located mainly at the C atom since the p states of C lie lower in energy with respect to the t_{2g} states of Sc. Since in total we have seven electrons and four are already accommodated in the spin-down bands, only three have to be accommodated in the spin-up band. Thus in the spin-up band again only the bonding hybrids with their main weight at the C atom are partially occupied and thus the spin moment is mainly concentrated at the sp -atom. As can be seen in the same graph the unoccupied states are mainly of Sc character since they are consisted of the antibonding $p - t_{2g}$ states and the localized e_g d -states of Sc. When we substitute V for Sc, the two extra electrons fill exclusively spin-up states since the half-metallicity is preserved and the Fermi level is again within the spin-down gap. Thus now all the bonding spin-up states are occupied and one electron occupies partially the localized spin-up e_g states of V (in total these states can occupy two electrons per spin). As a result the Fermi level falls within a large peak in the spin-up band and almost divides it in two equal parts. The spin-up peak of the e_g states is clearly separated by the antibonding $p - t_{2g}$ states as can be seen in the DOS. As a result of the above discussion V has now a spin magnetic moment of $\sim 1.19 \mu_B$ and C a spin magnetic moment of $\sim -0.19 \mu_B$ resulting to a total spin moment of $+1 \mu_B$ in agreement to the Slater-Pauling behavior. The spin moment of V can be decomposed to $1 \mu_B$ due to the e_g state, and $0.19 \mu_B$ which controbalances the $-0.19 \mu_B$ of C and come from the small imbalance in the distribution of the bonding $p - t_{2g}$ states between the two chemical species in the spin-up and spin-down bands. In the case of the Si compound the situation is similar with only noticeable difference the fact that Si carries in the case of ScSi a smaller absolute value of the spin magnetic moment with respect

to C in ScC while the situation is inversed when we compare the VSi to the VC alloy. ScSi and VSi compounds have significantly larger equilibrium lattice constants with respect to the ScC and VC alloys as shown in figure 1. Thus the hybridization between the Si p -states and the t_{2g} -states of Sc(V) is less intense than in the case of the C-based alloys resulting in bands which are more narrow in energy width but more intense (the scale in the vertical DOS axis in figure 3 is double for the Si-based alloys). Due to this small change in hybridization a variation in the spin magnetic moments occurs with respect to the C-based compounds.

We have also performed calculations for the intermediate concentrations x and in table 1 and figure 3 we have gathered the atom-resolved and total spin magnetic moments and DOS. The atom-resolved properties have been scaled to one atom. We have assumed that the lattice constants scale linearly with the concentration x between the perfect compounds as occurs experimentally for the quaternary Heusler alloys which have similar structure [19]. In order for these alloys to be half-metallic, the Slater-Pauling rule should be again valid where as valence of the transition-metal site we consider the $(1 - x) * Z_{Sc} + x * Z_V$, where $Z_{Sc} = 3$ and $Z_V = 5$ the valence of the Sc and V atoms respectively. As we dope ScC and ScSi with V, the bonding $p - t_{2g}$ states in the spin-up band start to move lower in energy with respect to the Fermi level and the peak of the e_g states starts appearing at the Fermi level as can be clearly seen for the case of $x = 0.8$. Thus almost all intermediate compounds follow the Slater-Pauling behavior as can be seen from the total spin moments in table 1 and the electronic and magnetic properties of the compounds vary in a continuous way with the concentration. The compounds are ferrimagnets since the V atoms have a spin moment antiparallel to the one of the Sc and C(Si) atoms.

The only exception of compounds which are not magnetic is the case of $[Sc_{1-x}V_x]C$ for $x = 0.4$ and 0.5 in the ZB lattice and $x = 0.5$ in the WZ structure. We will start our discussion from the case of $x = 0.5$. $[Sc_{0.5}V_{0.5}]C$ is not magnetic both in the ZB and WZ structures and as shown in the DOS presented in figure 3 it is actually a semiconductor since there are exactly eight valence electrons which occupy the bonding $p - t_{2g}$ states in both the spin-up and spin-down bands. The energy gap is about 0.4 eV. We can clearly distinguish in the DOS the occupied bonding hybrids, followed by the e_g bands just above the Fermi level with most of their weight at

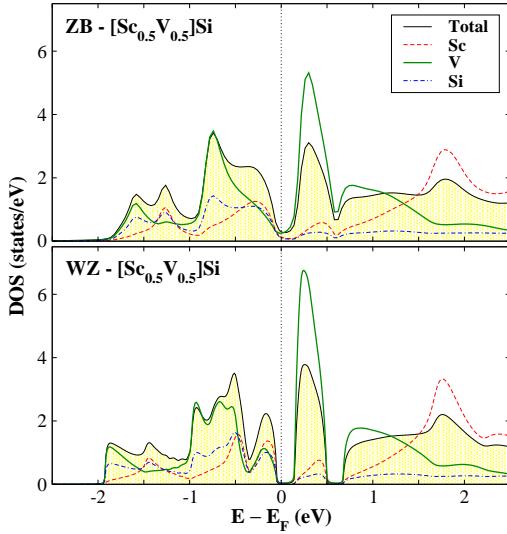


Fig. 4. (Color online) Total and atom-resolved DOS for $[Sc_{0.5}V_{0.5}]Si$ in both zincblende and wurtzite structures performing non-spinpolarized calculations. The atom-resolved DOS have been scaled to one atom.

the V atoms and which are clearly separated in energy from the antibonding $p - t_{2g}$ states which are even higher in energy (the deep-lying s states are not shown). In the case of $x = 0.4$ in the ZB structure the Fermi level falls in a region of small spin-up DOS (the DOS is not presented here) and due to the Stoner theorem the alloy is not magnetic contrary to the WZ structure where the Stoner theorem is satisfied even marginally resulting in a magnetic compound.

Contrary to $[Sc_{0.5}V_{0.5}]C$ the $[Sc_{0.5}V_{0.5}]Si$ alloy is magnetic and in reality it is a so-called half-metallic antiferromagnet [17,20] since the total spin-moment is exactly zero as in conventional antiferromagnets but the different constituents are magnetic as shown in table 1. The question which arises is why the Si-alloy shows such a different behavior from the C-alloy. To elucidate the origin of the difference we have performed non-magnetic calculations for the $[Sc_{0.5}V_{0.5}]Si$ alloy in both the ZB and WZ structures and we present the DOS in figure 4. The Fermi level falls within a deep of the DOS in the ZB structure and within a small gap in the WZ structure, thus due to Stoner theorem in both cases magnetism is not favorable. But Stoner theorem has a limited application in alloys where the situation is more complicated with respect to crystals made out of a single chemical element. Below the Fermi level the bands are concentrated in a small energy range and just above the Fermi level there is a very intense peak

due to the V e_g states making the non-magnetic solution unstable and the system prefers to be magnetic in order to lower its total energy.

4. Summary and conclusions

We have employed first-principles calculations and have studied the structural, electronic and magnetic properties of the $[Sc_{1-x}V_x]C$ and $[Sc_{1-x}V_x]Si$ alloys. In their equilibrium rocksalt structure all alloys are non-magnetic. The zincblende and wurtzite structures are degenerated with respect to the total energy and show magnetism. For all concentrations we found that the alloys in these two lattice structures are half-metallic with the gap located in the spin-down band. Moreover they are ferrimagnets since V and Sc atoms have antiparallel spin-magnetic moments. The total spin moment follows the Slater-Pauling behavior varying linearly between the $-1 \mu_B$ of the perfect ScC and $ScSi$ alloys and the $+1 \mu_B$ of the perfect VC and VSi alloys. At the critical concentration, both $[Sc_{0.5}V_{0.5}]C$ and $[Sc_{0.5}V_{0.5}]Si$ alloys present zero total spin-magnetic moment but the C-based alloy shows a semiconducting behavior since the Stoner criterion for magnetism is not satisfied. Contrary, the $[Sc_{0.5}V_{0.5}]Si$ compounds is a half-metallic antiferromagnet and thus very interesting for potential application in spintronics.

We have shown that also in the case of artificial binary compounds between transition-metal and sp atoms we can tune their magnetic properties in a continuous way by mixing atoms of neighboring chemical species. Following this procedure we were able to demonstrate the existence of half-metallic ferrimagnetism in the studied alloys (and in an extreme case even half-metallic antiferromagnetism) which is highly desirable for spintronic applications since ferrimagnets create smaller stray fields than ferromagnets and consequently lead to smaller energy losses in devices.

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